Pentadecane

629-62-9 | DTXSID6027268

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 10.3 °C

Global applicability domain: Inside

Local applicability domain index: 9.91e-01

Confidence level: 9.39e-01

Nearest Neighbors from the Training Set

Image not found

Pentadecane Measured: 9.90 Predicted: 10.3 Image not found

Hexadecane Measured: 18.1 Predicted: 16.9 Image not found

Tetradecane Measured: 5.80 Predicted: 3.94

Image not found

Heptadecane Measured: 22.0 Predicted: 22.2 Image not found

Tridecane
Measured: -5.30
Predicted: -4.65